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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	DEC 01	ChemPort single article sales feature unavailable
NEWS 3	APR 03	CAS coverage of exemplified prophetic substances enhanced
NEWS 4	APR 07	STN is raising the limits on saved answers
NEWS 5	APR 24	CA/CAplus now has more comprehensive patent assignee information
NEWS 6	APR 26	USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
NEWS 7	APR 28	CAS patent authority coverage expanded
NEWS 8	APR 28	ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS 9	APR 28	Limits doubled for structure searching in CAS REGISTRY
NEWS 10	MAY 08	STN Express, Version 8.4, now available
NEWS 11	MAY 11	STN on the Web enhanced
NEWS 12	MAY 11	BEILSTEIN substance information now available on STN Easy
NEWS 13	MAY 14	DGENE, PCTGEN and USGENE enhanced with increased limits for exact sequence match searches and introduction of free HIT display format
NEWS 14	MAY 15	INPADOCDB and INPAFAMDB enhanced with Chinese legal status data
NEWS 15	MAY 28	CAS databases on STN enhanced with NANO super role in records back to 1992
NEWS 16	JUN 01	CAS REGISTRY Source of Registration (SR) searching enhanced on STN
NEWS 17	JUN 26	NUTRACEUT and PHARMAML no longer updated
NEWS 18	JUN 29	IMSCOPROFILE now reloaded monthly
NEWS 19	JUN 29	EPFULL adds SLART to AB, MCLM, and TI fields

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items

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and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:49:16 ON 08 JUL 2009

=> fil reg
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 0.22 | 0.22

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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 7 JUL 2009 HIGHEST RN 1161069-81-3
DICTIONARY FILE UPDATES: 7 JUL 2009 HIGHEST RN 1161069-81-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

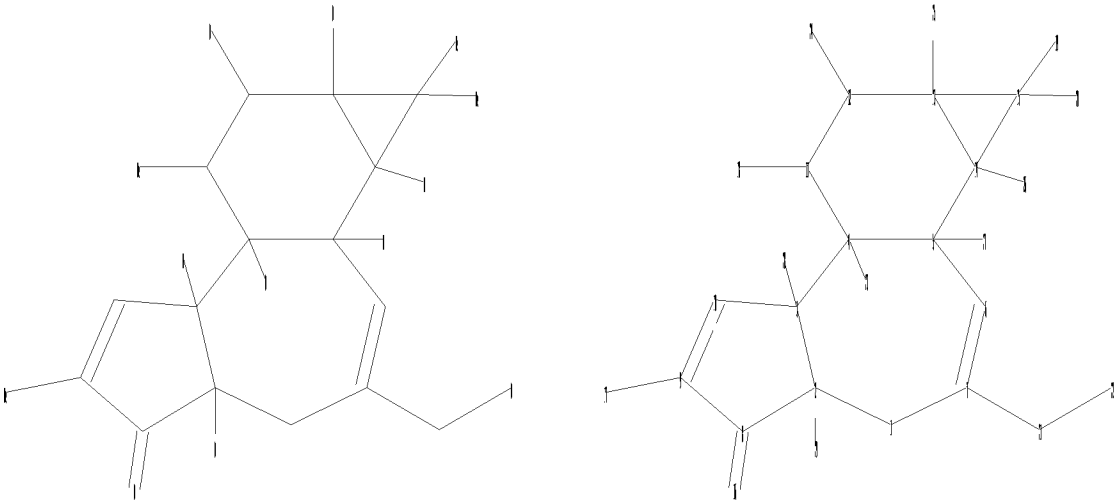
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\STNEXP\Queries\10557922 generic.str



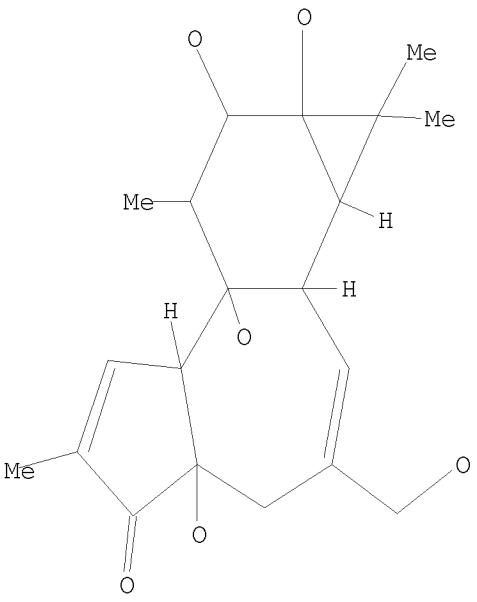
chain nodes :
16 17 18 19 20 21 22 23 24 25 26 27 28 29
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :

2-29 3-28 4-23 5-27 7-21 8-16 9-17 11-18 12-24 13-25 14-26 15-19 15-20
21-22
ring bonds :
1-2 1-7 2-3 2-8 3-4 3-10 4-5 4-11 5-6 5-14 6-7 8-9 9-10 11-12 12-13
13-14 13-15 14-15
exact/norm bonds :
1-2 1-7 2-3 2-8 2-29 3-4 3-10 4-5 4-11 4-23 5-6 5-14 6-7 8-9 8-16
9-10 11-12 12-13 12-24 13-14 13-15 13-25 14-15 21-22
exact bonds :
3-28 5-27 7-21 9-17 11-18 14-26 15-19 15-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS
 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS

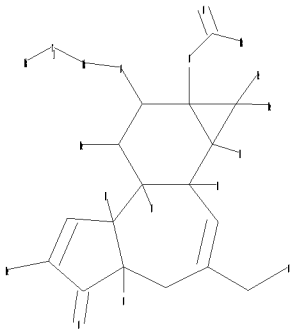
L1   STRUCTURE UPLOADED

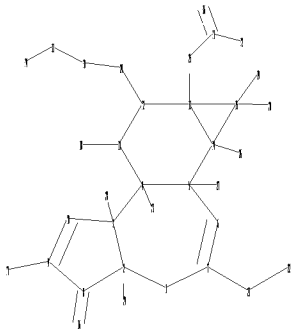
=> d l1
L1 HAS NO ANSWERS
L1   STR



Structure attributes must be viewed using STN Express query preparation.

=>
Uploading C:\Program Files\STNEXP\Queries\10557922 sub a.str





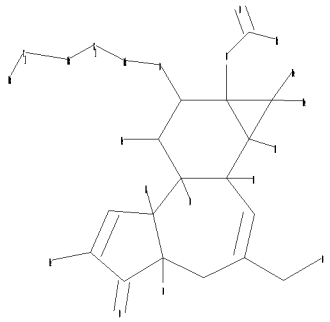
chain nodes :
16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 36
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
2-29 3-28 4-23 5-27 7-21 8-16 9-17 11-18 12-24 13-25 14-26 15-19 15-20
21-22 24-30 25-31 30-33 31-32 31-36 33-34
ring bonds :
1-2 1-7 2-3 2-8 3-4 3-10 4-5 4-11 5-6 5-14 6-7 8-9 9-10 11-12 12-13
13-14 13-15 14-15
exact/norm bonds :
1-2 1-7 2-3 2-8 2-29 3-4 3-10 4-5 4-11 4-23 5-6 5-14 6-7 8-9 8-16
9-10 11-12 12-13 12-24 13-14 13-15 13-25 14-15 21-22 24-30 25-31 30-33
31-32 31-36 33-34
exact bonds :
3-28 5-27 7-21 9-17 11-18 14-26 15-19 15-20

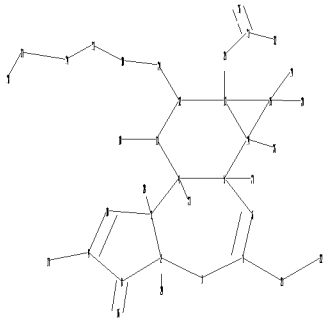
G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 36:CLASS

L2 STRUCTURE UPLOADED

=>
Uploading C:\Program Files\STNEXP\Queries\10557922 sub b.str





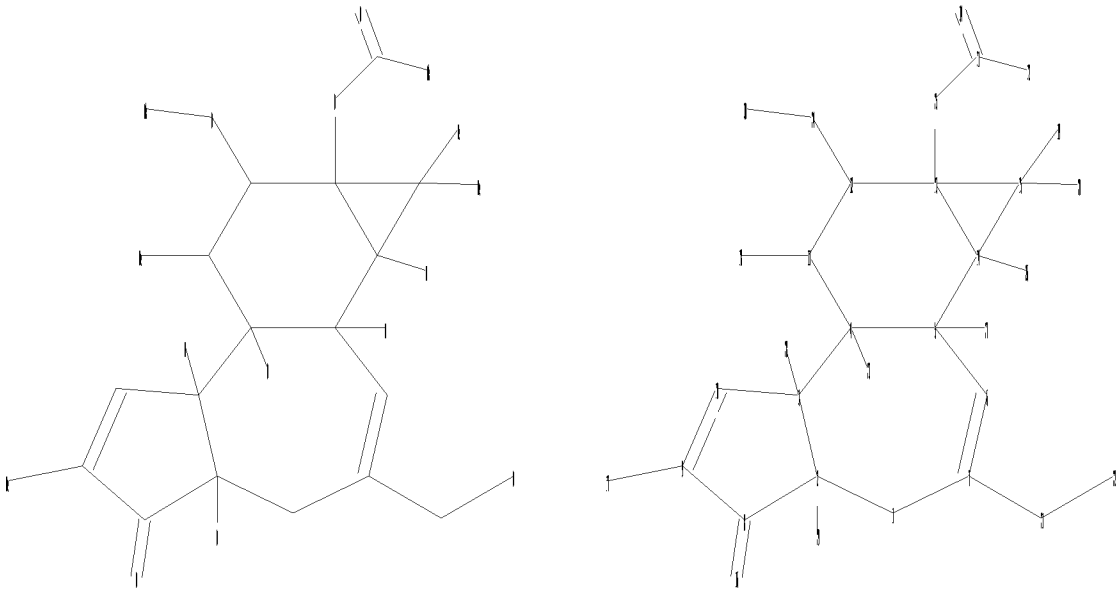
chain nodes :
16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 36 37
38
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
2-29 3-28 4-23 5-27 7-21 8-16 9-17 11-18 12-24 13-25 14-26 15-19 15-20
21-22 24-30 25-31 30-33 31-32 31-36 33-34 34-37 37-38
ring bonds :
1-2 1-7 2-3 2-8 3-4 3-10 4-5 4-11 5-6 5-14 6-7 8-9 9-10 11-12 12-13
13-14 13-15 14-15
exact/norm bonds :
1-2 1-7 2-3 2-8 2-29 3-4 3-10 4-5 4-11 4-23 5-6 5-14 6-7 8-9 8-16
9-10 11-12 12-13 12-24 13-14 13-15 13-25 14-15 21-22 24-30 25-31 30-33
31-32 31-36 33-34 34-37 37-38
exact bonds :
3-28 5-27 7-21 9-17 11-18 14-26 15-19 15-20

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 36:CLASS
37:CLASS 38:CLASS

L3 STRUCTURE UPLOADED

=>
Uploading C:\Program Files\STNEXP\Queries\10557922 sub c.str



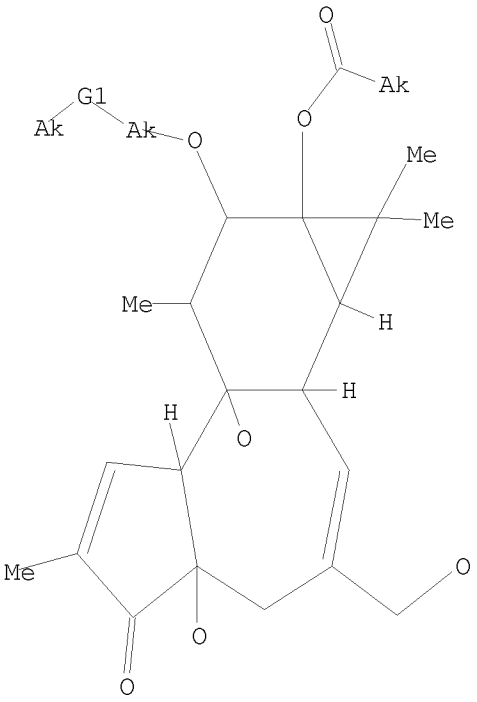
chain nodes :
16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 34
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
2-29 3-28 4-23 5-27 7-21 8-16 9-17 11-18 12-24 13-25 14-26 15-19 15-20
21-22 24-30 25-31 31-32 31-34
ring bonds :
1-2 1-7 2-3 2-8 3-4 3-10 4-5 4-11 5-6 5-14 6-7 8-9 9-10 11-12 12-13
13-14 13-15 14-15
exact/norm bonds :
1-2 1-7 2-3 2-8 2-29 3-4 3-10 4-5 4-11 4-23 5-6 5-14 6-7 8-9 8-16
9-10 11-12 12-13 12-24 13-14 13-15 13-25 14-15 21-22 24-30 25-31 31-32
31-34
exact bonds :
3-28 5-27 7-21 9-17 11-18 14-26 15-19 15-20

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 34:CLASS

L4 STRUCTURE UPLOADED

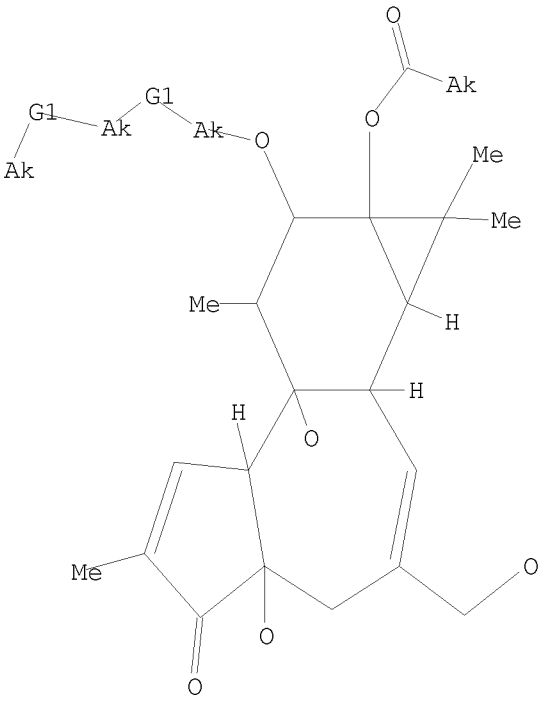
=> d l2
L2 HAS NO ANSWERS
L2 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

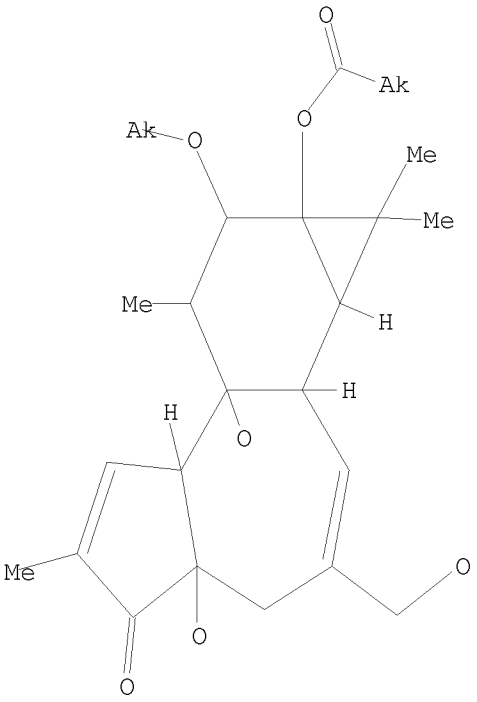
=> d l3
L3 HAS NO ANSWERS
L3 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> d l4
L4 HAS NO ANSWERS
L4 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 sss ful
FULL SEARCH INITIATED 14:51:55 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1569 TO ITERATE

100.0% PROCESSED     1569 ITERATIONS                             791 ANSWERS
SEARCH TIME: 00.00.01

L5          791 SEA SSS FUL L1

=> s l2 sub=l5 sss ful
FULL SUBSET SEARCH INITIATED 14:52:10 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -      672 TO ITERATE

100.0% PROCESSED      672 ITERATIONS                              18 ANSWERS
SEARCH TIME: 00.00.01

L6           18 SEA SUB=L5 SSS FUL L2

=> s l3 sub=l5 sss ful
FULL SUBSET SEARCH INITIATED 14:52:19 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -      672 TO ITERATE

100.0% PROCESSED      672 ITERATIONS                               6 ANSWERS
SEARCH TIME: 00.00.01

L7            6 SEA SUB=L5 SSS FUL L3

=> s l4 sub=l5 sss ful
FULL SUBSET SEARCH INITIATED 14:52:23 FILE 'REGISTRY'
```

FULL SUBSET SCREEN SEARCH COMPLETED - 732 TO ITERATE

100.0% PROCESSED 732 ITERATIONS 596 ANSWERS
SEARCH TIME: 00.00.01

L8 596 SEA SUB=L5 SSS FUL L4

=> fil cap
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 319.80 320.02

FILE 'CAPLUS' ENTERED AT 14:52:30 ON 08 JUL 2009
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FILE COVERS 1907 - 8 Jul 2009 VOL 151 ISS 2
FILE LAST UPDATED: 7 Jul 2009 (20090707/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

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http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 14:49:16 ON 08 JUL 2009)

FILE 'REGISTRY' ENTERED AT 14:49:40 ON 08 JUL 2009
L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 STRUCTURE UPLOADED
L4 STRUCTURE UPLOADED
L5 791 S L1 SSS FUL
L6 18 S L2 SSS FUL SUB=L5
L7 6 S L3 SSS FUL SUB=L5
L8 596 S L4 SSS FUL SUB=L5

FILE 'CAPLUS' ENTERED AT 14:52:30 ON 08 JUL 2009

=> s l6 or l7 or l8
6 L6
4 L7

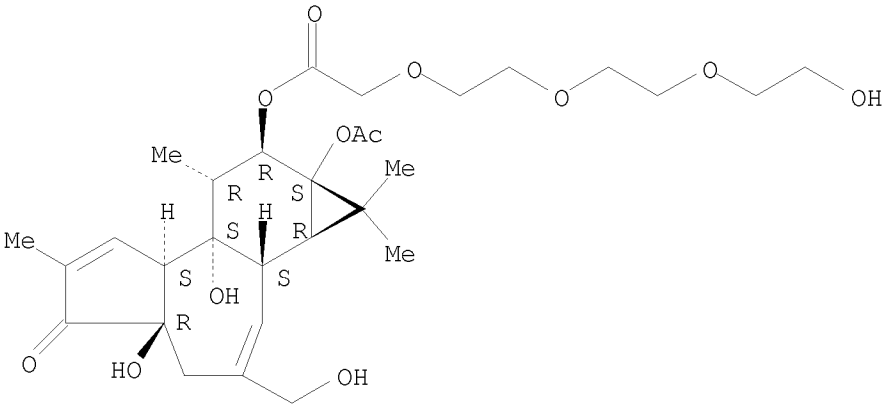
```
         14990 L8
L9       14990 L6 OR L7 OR L8

=> s l6 or l7
             6 L6
             4 L7
L10          6 L6 OR L7

=> d l10 1-6 ibib abs hitstr

L10  ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         2006:1330269  CAPLUS
DOCUMENT NUMBER:          147:294460
TITLE:                    Identification of potent, selective protein kinase C
                          inhibitors based on a phorbol skeleton
AUTHOR(S):                Yamatsugu, Kenzo; Motoki, Rie; Kanai, Motomu;
                          Shibasaki, Masakatsu
CORPORATE SOURCE:         Graduate School of Pharmaceutical Sciences, The
                          University of Tokyo, Hongo, Bunkyo-ku, Tokyo,
                          113-0033, Japan
SOURCE:                   Chemistry--An Asian Journal (2006), 1(3), 314-321
                          CODEN: CAAJBI; ISSN: 1861-4728
PUBLISHER:                Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 147:294460
AB   The elucidation of specific functions of protein kinase C (PKC) subtypes
     in physiol. processes is an important challenge for the future development
     of new drug targets.  Subtype-selective PKC agonists and antagonists are
     useful biol. tools for this purpose.  Most of the currently used PKC
     modulators elicit their activities through binding to the ATP binding site
     of PKC, which shares many features with other kinases.  PKC modulators
     that target the PKC regulatory domain are considered to be advantageous in
     terms of selectivity, because the structure of the regulatory domain is
     intrinsic to each PKC subtype.  In this paper, we describe the
     identification of new potent and conventional PKC-selective inhibitors
     that target the regulatory domain.  The inhibitors contain a phorbol
     skeleton, a naturally occurring potent and selective PKC regulatory domain
     binder, with a perfluorinated alkyl group and a polyether hydrophilic
     chain on a terephthaloyl aromatic ring at the C12 position.  Both of these
     substituents are essential for the potent inhibitory activity.
     Specifically, the binding affinity between PKC and the phorbol ester
     analogs was improved by an electron-deficient aromatic ring at C12.  This
     finding cannot be explained by the previously proposed binding model and
     suggests a new binding mode between phorbol esters and PKC.
IT   947338-37-6
     RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
     (Biological study)
        (phorbol skeleton based potent, selective protein kinase C inhibitors)
RN   947338-37-6  CAPLUS
CN   Acetic acid, 2-[2-[2-(2-hydroxyethoxy)ethoxy]ethoxy]-,
     (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-9a-(acetyloxy)-1a,1b,4,4a,5,7a,7b,8,9,9a-
     decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-1H-
     cyclopropa[3,4]benz[1,2-e]azulen-9-yl ester  (CA INDEX NAME)

Absolute stereochemistry.
```



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1157380 CAPLUS
DOCUMENT NUMBER: 144:31978
TITLE: Novel phorbol esters exert dichotomous effects on inhibition of HIV-1 infection and activation of latent HIV-1 expression
AUTHOR(S): Zhong, Yu; Matsuya, Yuji; Nemoto, Hideo; Mori, Masao; Saito, Haruo; Yamamoto, Naoki
CORPORATE SOURCE: Department of Molecular Virology, Bio-Response, Graduate School, Tokyo Medical and Dental University, Tokyo, Japan
SOURCE: Antiviral Chemistry & Chemotherapy (2005), 16(5), 303-313
CODEN: ACCHEH; ISSN: 0956-3202
PUBLISHER: International Medical Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two new phorbol esters, NPB-11 (12-O-methoxymethylphorbol-13-decanoate) and NPB-15 (12-O-benzyloxymethylphorbol-13-decanoate) were synthesized. The compds. exhibited potent anti-HIV-1 activity and low cytotoxicity in MT-4 cells by MTT assay even at a high concentration [50% cytotoxic concns. (CC50) were 8.32 and 4.39 μg/mL, resp.]. Two inhibitors strongly suppressed HIV-1 (IIIB strain) replication in MT-4 cells with a 50% effective concentration (EC50) of 1.3 and 0.27 ng/mL, resp. NPB-11 efficiently blocked replication of both X4 and R5 HIV-1 in PHA-activated peripheral blood mononuclear cells and MT-4 cells as revealed by p24 assay. The antiviral activity appeared to be mediated, at least partially, by the down-regulation of the expression of CD4 and the HIV-1 co-receptors, CXCR4 and CCR5. The compds. were also capable of selectively up-regulating HIV-1 expression in a variety of latently infected cell lines and inducing cell death in HIV-1 infected cells. The effect of NPBs on the induction of HIV-1 was specifically blocked by nontoxic doses of a protein kinase C blocker, staurosporine. NPB-11 blocked the spread of HIV-1 released from latently infected ACH-2 cells to MT-4 cells in a co-culture system. When combined with AZT, NPB-11 synergistically inhibited HIV-1 replication in MTT assay using MT-4 cells. These data suggest that these agents might be useful in reducing persistent viral reservoirs in patients and as adjuvant therapy in patients treated with HAART.

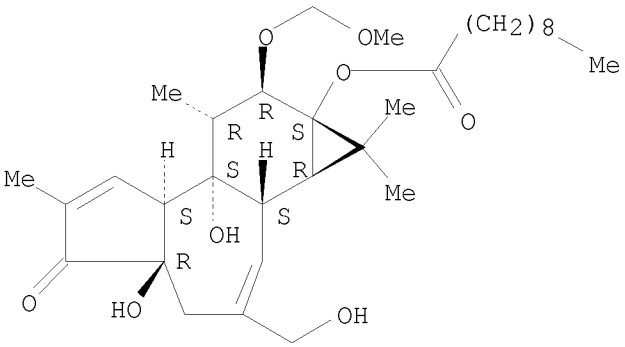
IT 800385-91-5, NPB 11 859528-10-2, NPB 15
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel phorbol esters exert dichotomous effects on inhibition of HIV-1

infection and activation of latent HIV-1 expression)

RN 800385-91-5 CAPLUS

CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-1,1a,1b,4,4a,5,7a,7b,9,9-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-9-(methoxymethoxy)-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

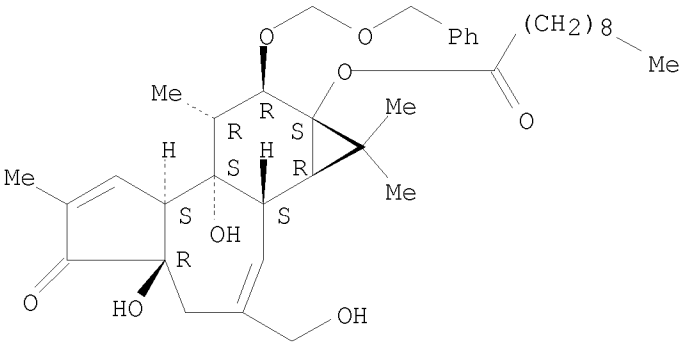
Absolute stereochemistry.



RN 859528-10-2 CAPLUS

CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-9-[(phenylmethoxy)methoxy]-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:520769 CAPLUS

DOCUMENT NUMBER: 143:145807

TITLE: Synthesis of new phorbol derivatives having ethereal side chain and evaluation of their anti-HIV activity

AUTHOR(S): Matsuya, Yuji; Yu, Zhong; Yamamoto, Naoki; Mori, Masao; Saito, Haruo; Takeuchi, Makoto; Ito, Mamiko; Nemoto, Hideo

CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Toyama Medical and Pharmaceutical University, Toyama, 930-0914, Japan

SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(14), 4383-4388
CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

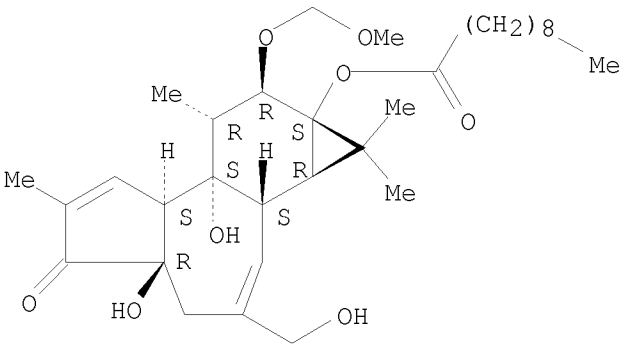
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:145807

AB Several new phorbol derivs. having ethereal substituents at the 12-position were synthesized and subjected to biol. evaluation to find new candidates of an anti-HIV agent. Among them, 12-O-(methoxymethyl)phorbol 13-decanoate showed potent inhibitory activity against infection of HIV-1 in MT-4 cells (EC50: 1.3 ng/mL) and relatively low cytotoxicity (CC50: 8.3 μg/mL). This compound was also found to have sufficient stability in mouse plasma compared with the corresponding 12-acetate derivative, which was an equipotent HIV-1 inhibitor, but with an activity that decreased considerably after plasma treatment.

IT 800385-91-5P 800385-92-6P 859528-10-2P
859528-11-3P, 12-O-Methoxymethyl-20-O-methylphorbol 13-decanoate
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of new phorbol derivs. having ethereal side chain and evaluation of their anti-HIV activity)

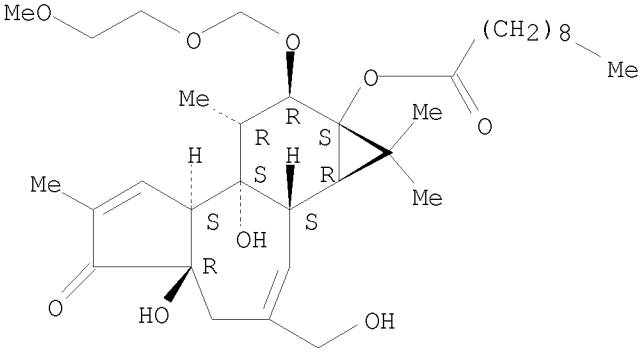
RN 800385-91-5 CAPLUS
CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-1,1a,1b,4,4a,5,7a,7b,9,9-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-9-(methoxymethoxy)-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



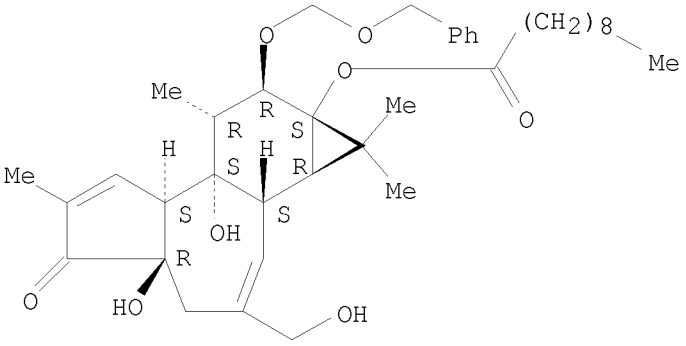
RN 800385-92-6 CAPLUS
CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-1,1a,1b,4,4a,5,7a,7b,9,9-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-9-[(2-methoxyethoxy)methoxy]-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



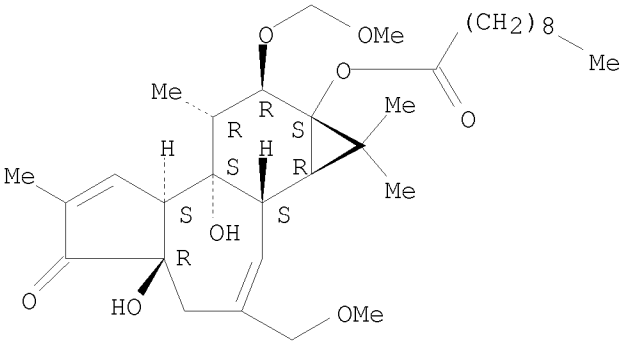
RN 859528-10-2 CAPLUS
CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-9-[(phenylmethoxy)methoxy]-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 859528-11-3 CAPLUS
CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-4a,7b-dihydroxy-9-(methoxymethoxy)-3-(methoxymethyl)-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



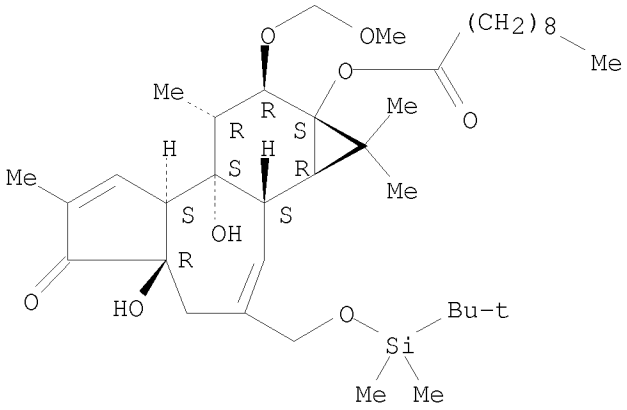
IT 800385-87-9P 800385-88-0P 859528-09-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(synthesis of new phorbol derivs. having ethereal side chain and evaluation of their anti-HIV activity)

RN 800385-87-9 CAPLUS

CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-1,1a,1b,4,4a,5,7a,7b,9,9-decahydro-4a,7b-dihydroxy-9-(methoxymethoxy)-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

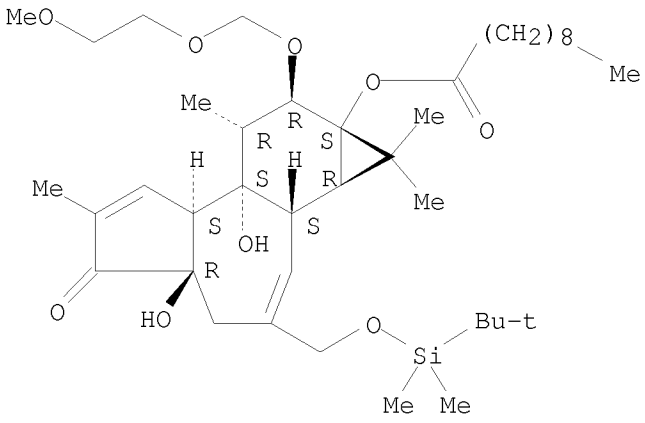
Absolute stereochemistry.



RN 800385-88-0 CAPLUS

CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-4a,7b-dihydroxy-9-[(2-methoxyethoxy)methoxy]-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (CA INDEX NAME)

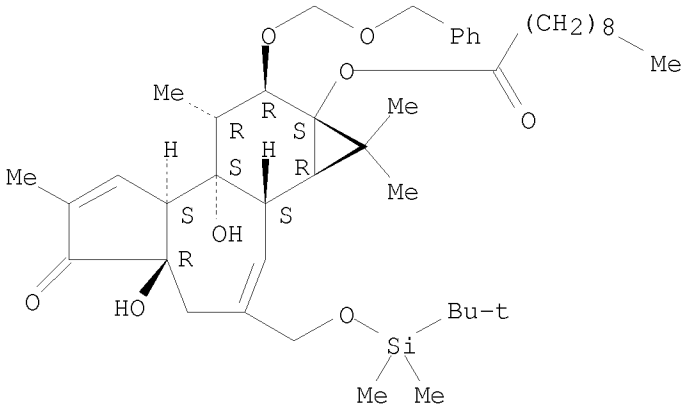
Absolute stereochemistry.



RN 859528-09-9 CAPLUS

CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-4a,7b-dihydroxy-1,1,6,8-tetramethyl-5-oxo-9-[(phenylmethoxy)methoxy]-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

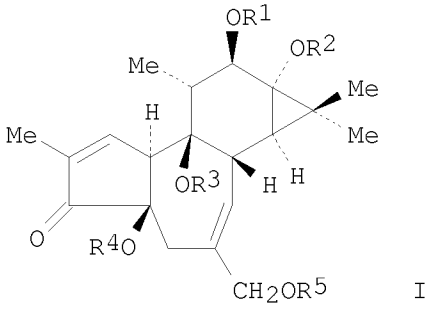


REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:1036894 CAPLUS
DOCUMENT NUMBER: 142:16778
TITLE: Compounds and preparations having antiviral effect
INVENTOR(S): Mori, Masao; Saito, Haruo; Nemoto, Hideo; Yamamoto, Naoki; Hattori, Masao
PATENT ASSIGNEE(S): Lead Chemical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004103360	A1	20041202	WO 2003-JP6422	20030522
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003242405	A1	20041213	AU 2003-242405	20030522
US 20070066684	A1	20070322	US 2005-557922	20051222

PRIORITY APPLN. INFO.: WO 2003-JP6422 A 20030522
OTHER SOURCE(S): MARPAT 142:16778
GI



I

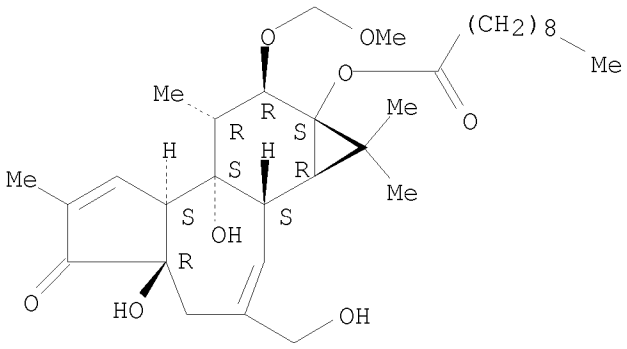
AB Antiviral prepns. containing, as the active ingredient, phorbol derivs. which are represented by the following general formula I: wherein R1 represents -CH2aX(CH2)bCH3, -CH2cX(CH2)dYCH3, -CO(CH2)eCH3or -(CH2)fCH3; R2 represents -CO(CH2)nCH3; and R3, R4 and R5 represent each hydrogen or aliphatic or aromatic carboxylate (wherein X and Y are each O or S; and a to f and n stand for each a numerical value); and show a specific safety index S.I. = EC50/EC50 (i.e., a ratio of the concentration at which HIV-1-induced cytopathogenic effect (CPE) in MT-4 cells is inhibited by 50% to the concentration at which the survival of MT-4 cells is lowered by 50% in a cell proliferation test) of 10 or more. These prepns. are efficacious particularly against human immunodeficiency virus (HIV).

IT 800385-91-5P 800385-92-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(phorbol compds. and prepns. having antiviral effect against HIV)

RN 800385-91-5 CAPLUS

CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-1,1a,1b,4,4a,5,7a,7b,9,9-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-9-(methoxymethoxy)-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

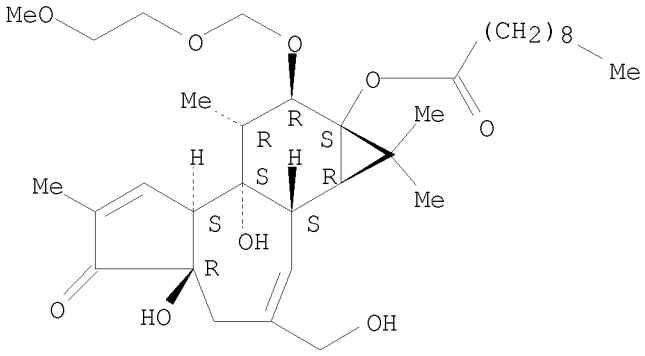
Absolute stereochemistry.



RN 800385-92-6 CAPLUS

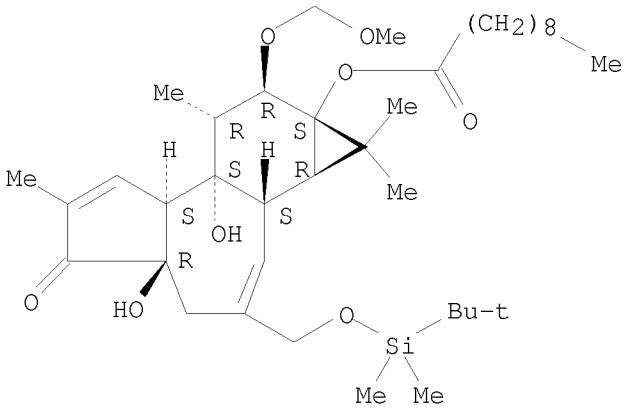
CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-1,1a,1b,4,4a,5,7a,7b,9,9-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-9-[(2-methoxyethoxy)methoxy]-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



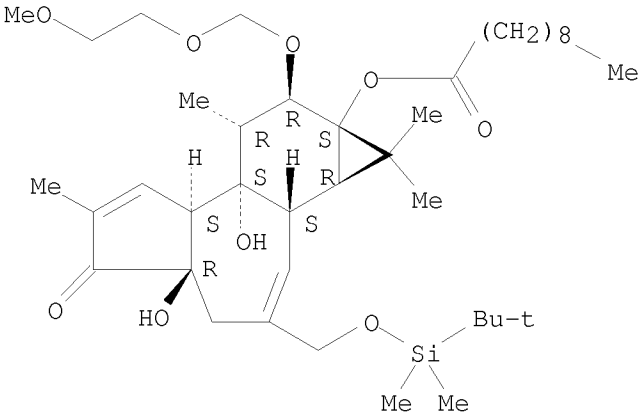
IT 800385-87-9P 800385-88-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(phorbol compds. and prepns. having antiviral effect against HIV)
RN 800385-87-9 CAPLUS
CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-1,1a,1b,4,4a,5,7a,7b,9,9-decahydro-4a,7b-dihydroxy-9-(methoxymethoxy)-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



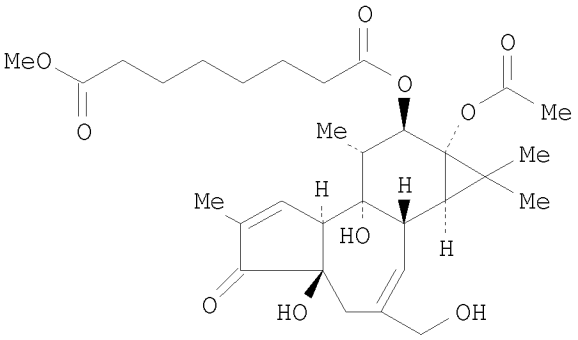
RN 800385-88-0 CAPLUS
CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-4a,7b-dihydroxy-9-[(2-methoxyethoxy)methoxy]-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:391368 CAPLUS
DOCUMENT NUMBER: 139:117559
TITLE: Protein Kinase C Translocation by Modified Phorbol Esters with Functionalized Lipophilic Regions
AUTHOR(S): Bertolini, Thomas M.; Giorgione, Jennifer; Harvey, Daniel F.; Newton, Alexandra C.
CORPORATE SOURCE: Departments of Chemistry and Pharmacology, University of California, La Jolla, CA, 92093, USA
SOURCE: Journal of Organic Chemistry (2003), 68(13), 5028-5036
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:117559
GI



I

AB Several novel phorbol esters, e.g., I, were prepared with polar functional groups terminating their C12 and/or C13 acyl chains. Designed to be inhibitory protein kinase C (PKC) ligands, these phorbol analogs contain various polar functional groups (amide, ester, carboxylic acid, or quaternary ammonium salt) to prevent membrane insertion of the PKC-phorbol ester complex. All phorbol derivs. were synthesized with use of diterpene starting materials obtained from croton oil, the seed oil of Croton tiglium. The ability of these derivs. to recruit PKC to the lipid

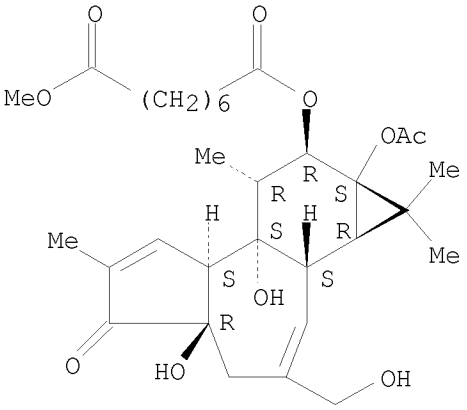
bilayer-a usual requirement for enzyme activation-was determined by using a sucrose-loaded vesicle assay. Phorbol 12-octanoate-13-acetate derivs. translocate PKC-βII to increasing degrees as the functionality on the C12 ester becomes more hydrophobic. Likewise, PKC translocation by carboxylic acid-containing phorbol esters was dependent upon length and saturation of the hydrocarbon tether. The most promising PKC inhibitors had short carboxylic acids capping their C12 and C13 acyl chains, since these compds. did not recruit PKC to any appreciable extent.

IT 561063-09-0P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and protein kinase C translocation studies of phorbol esters)

RN 561063-09-0 CAPLUS

CN Octanedioic acid, 1-[(1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-9a-(acetyloxy)-1a,1b,4,4a,5,7a,7b,8,9,9a-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-1H-cyclopropa[3,4]benz[1,2-e]azulen-9-yl] 8-methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

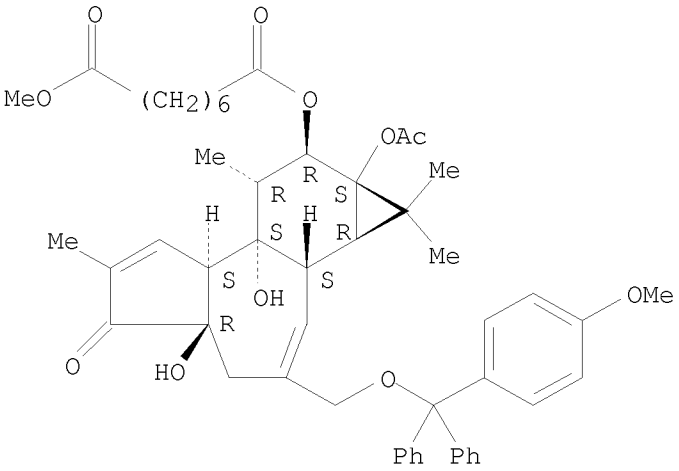


IT 561063-24-9P 561063-29-4P 561063-32-9P
561063-34-1P 561063-40-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and protein kinase C translocation studies of phorbol esters)

RN 561063-24-9 CAPLUS

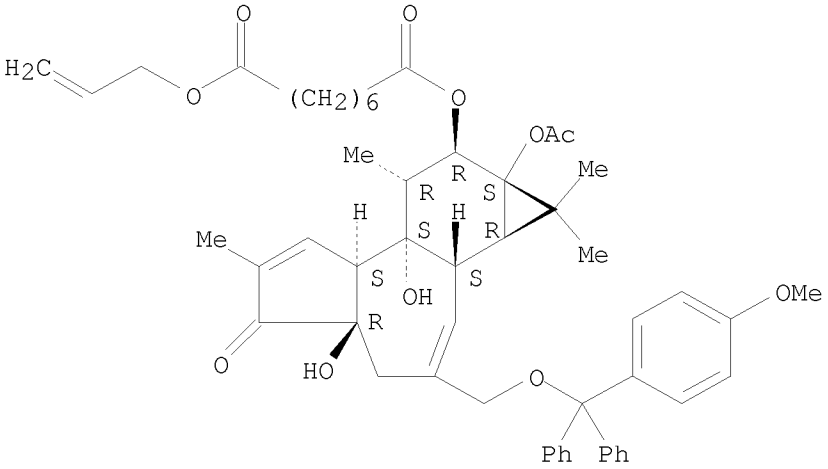
CN Octanedioic acid, 1-[(1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-9a-(acetyloxy)-1a,1b,4,4a,5,7a,7b,8,9,9a-decahydro-4a,7b-dihydroxy-3-[[(4-methoxyphenyl)diphenylmethoxy]methyl]-1,1,6,8-tetramethyl-5-oxo-1H-cyclopropa[3,4]benz[1,2-e]azulen-9-yl] 8-methyl ester (CA INDEX NAME)

Absolute stereochemistry.



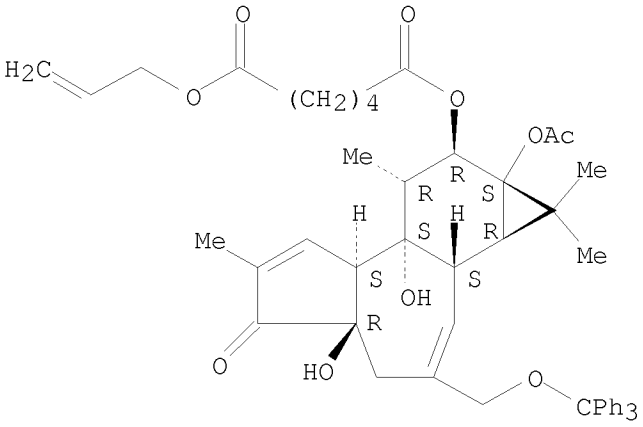
RN 561063-29-4 CAPLUS
CN Octanedioic acid, 1-[(1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-9a-(acetyloxy)-1a,1b,4,4a,5,7a,7b,8,9,9a-decahydro-4a,7b-dihydroxy-3-[[(4-methoxyphenyl)diphenylmethoxy]methyl]-1,1,6,8-tetramethyl-5-oxo-1H-cyclopropa[3,4]benz[1,2-e]azulen-9-yl] 8-(2-propen-1-yl) ester (CA INDEX NAME)

Absolute stereochemistry.



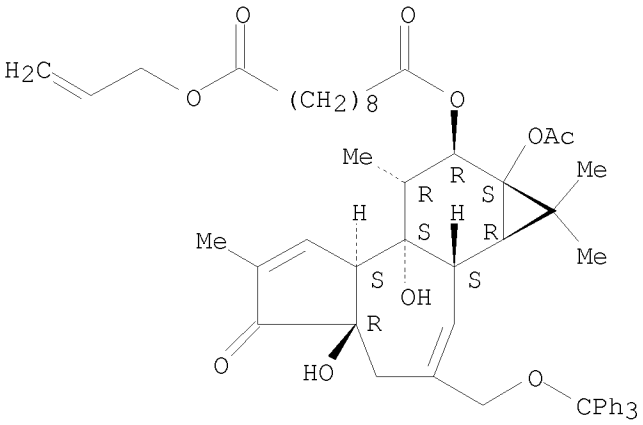
RN 561063-32-9 CAPLUS
CN Hexanedioic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-9a-(acetyloxy)-1a,1b,4,4a,5,7a,7b,8,9,9a-decahydro-4a,7b-dihydroxy-1,1,6,8-tetramethyl-5-oxo-3-[(triphenylmethoxy)methyl]-1H-cyclopropa[3,4]benz[1,2-e]azulen-9-yl 2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



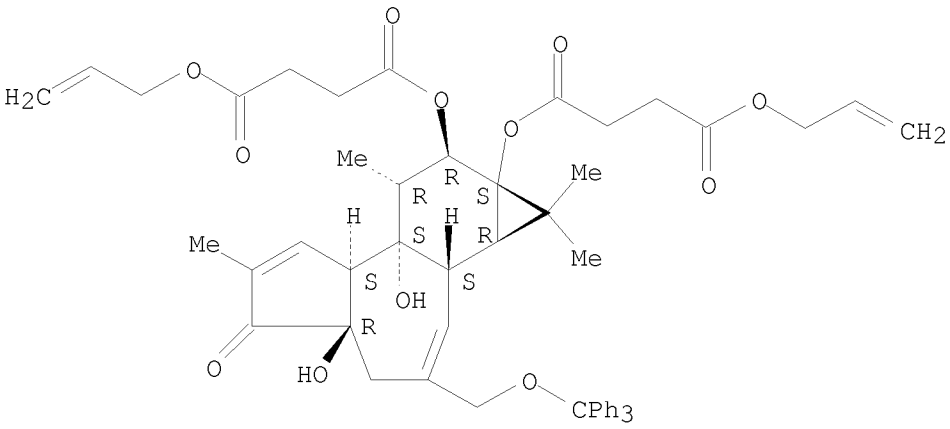
RN 561063-34-1 CAPLUS
CN Decanedioic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-9a-(acetyloxy)-1a,1b,4,4a,5,7a,7b,8,9,9a-decahydro-4a,7b-dihydroxy-1,1,6,8-tetramethyl-5-oxo-3-[(triphenylmethoxy)methyl]-1H-cyclopropa[3,4]benz[1,2-e]azulen-9-yl 2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 561063-40-9 CAPLUS
CN Butanedioic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-4a,7b-dihydroxy-1,1,6,8-tetramethyl-5-oxo-3-[(triphenylmethoxy)methyl]-9aH-cyclopropa[3,4]benz[1,2-e]azulene-9,9a-diyl di-2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:550357 CAPLUS
DOCUMENT NUMBER: 131:310739
TITLE: Mapping phorbol ester binding domains of protein kinase C (PKC). The design, synthesis, and biological activity of novel phorbol ester dimers
AUTHOR(S): Wender, Paul A.; Koehler, Michael F. T.; Wright, Dennis L.; Irie, Kazuhiro
CORPORATE SOURCE: Dep. Chemistry, Stanford Univ., Stanford, CA, 94305, USA
SOURCE: Synthesis (1999), (Spec. Iss.), 1401-1406
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:310739

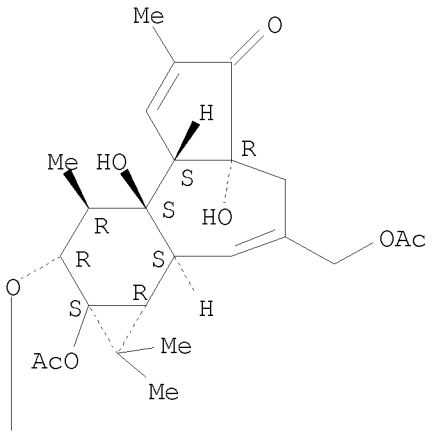
AB The design and synthesis of a new class of protein kinase C (PKC) activators, phorbol ester dimers, is described. These dimers bind to and activate PKC with affinities depending dramatically on their tether length and composition In two cases, the binding affinities of these novel compds. exceeded that of phorbol dibutyrate.

IT 247226-59-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and protein kinase C inhibition of phorbol ester dimers)

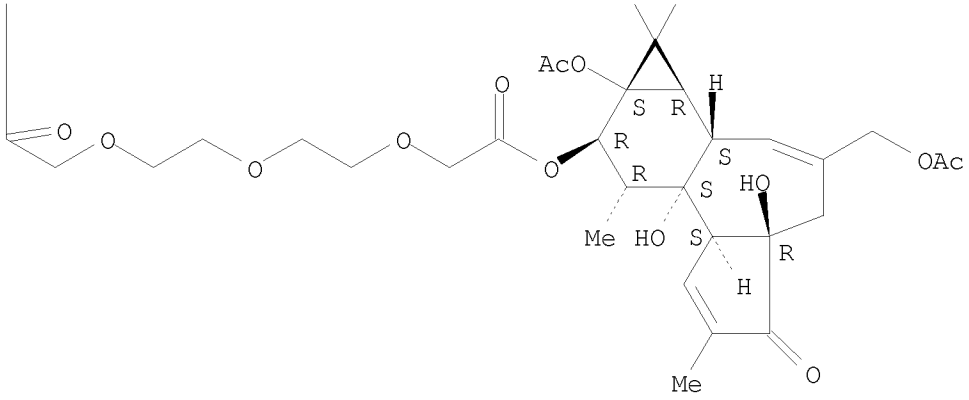
RN 247226-59-1 CAPLUS
CN Acetic acid, 2,2'-[oxybis(2,1-ethanediyloxy)]bis-, bis[(1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-9a-(acetyloxy)-3-[(acetyloxy)methyl]-1a,1b,4,4a,5,7a,7b,8,9,9a-decahydro-4a,7b-dihydroxy-1,1,6,8-tetramethyl-5-oxo-1H-cyclopropa[3,4]benz[1,2-e]azulen-9-yl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



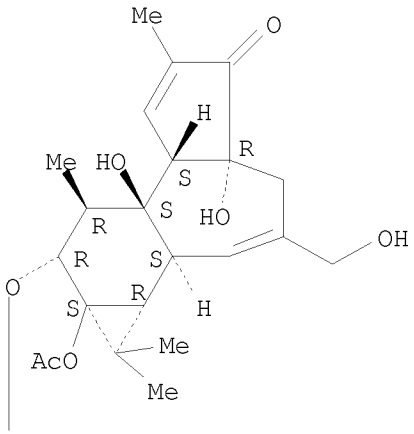
PAGE 2-A

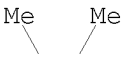


IT 247226-63-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and protein kinase C inhibition of phorbol ester dimers)
RN 247226-63-7 CAPLUS
CN Acetic acid, 2,2'-[oxybis(2,1-ethanediyloxy)]bis-,
bis[(1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-9a-(acetyloxy)-
1a,1b,4,4a,5,7a,7b,8,9,9a-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-
1,1,6,8-tetramethyl-5-oxo-1H-cyclopropa[3,4]benz[1,2-e]azulen-9-yl] ester
(9CI) (CA INDEX NAME)

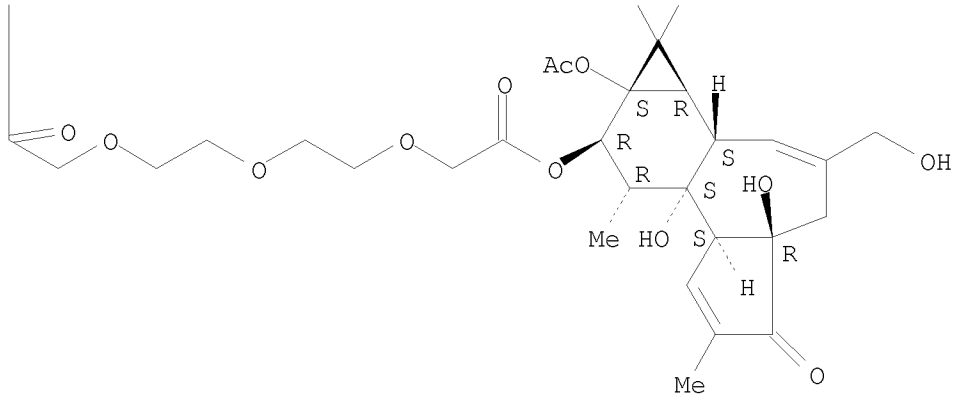
Absolute stereochemistry.

PAGE 1-A





PAGE 2-A



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            111 HIVS
          85642 HIV
                (HIV OR HIVS)
L12         182 L11 AND HIV

=> s l12 and (py<2003 or ay<2003 or pry<2003)
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       4508261 AY<2003
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L13         153 L12 AND (PY<2003 OR AY<2003 OR PRY<2003)

=> d l13 ibib abs hitstr

L13  ANSWER 1 OF 153  CAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         2004:270090  CAPLUS
DOCUMENT NUMBER:          140:302344
TITLE:                    Methods for assessing the ability of HIV
                          patients to restrict HIV replication
INVENTOR(S):              Connors, Mark; Migueles, Stephen A.
PATENT ASSIGNEE(S):       The Government of the United States of America, as
                          Represented by the Secretary Department of Health and
                          Human Services, USA
SOURCE:                   PCT Int. Appl., 81 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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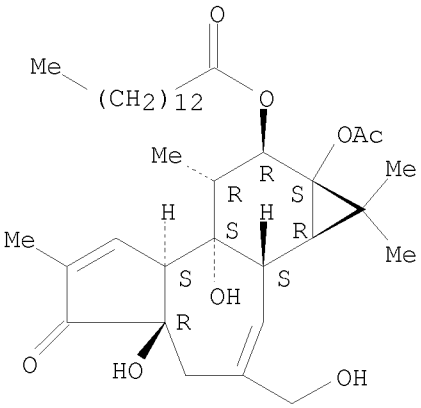
     WO 2004027034         A2    20040401    WO 2003-US29549         20030922 <--
     WO 2004027034         A3    20050602
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2003275044         A1    20040408    AU 2003-275044          20030922 <--
PRIORITY APPLN. INFO.:                     US 2002-412020P     P    20020920 <--
                                           WO 2003-US29549     W    20030922

AB   The authors disclose methods for evaluating the effectiveness of
     HIV therapies and vaccines and methods for assessing the ability
     of HIV patients to restrict virus replication.  Upon
     restimulation of CD8+ T cells or peripheral blood mononuclear cells from a
     patient, proliferation of the CD8+ T cells, the expression of perforin in
     these cells, and the cell cycle stage of these cells may be measured and
     used as in vitro markers for monitoring the patient's ability to restrict
     HIV replication and the effectiveness of the therapies and
     vaccines applied.  Significant proliferation of CD8+ T cell, the presence
     of perforin in these cells, and the ability of these cells to progress
     beyond the G1 stage signify the patient's ability to restrict HIV
     replication and a favorable effect of the therapies or vaccines.  These
     methods may be advantageously applied in conjunction with other
     measurements of HIV specific immune response.
IT   16561-29-8, Phorbol-12-myristate-13-acetate
     RL: BUU (Biological use, unclassified); BIOL (Biological study); USES
     (Uses)
        (for expansion of CD8+ T-cells in culture in relation to resistance to
        HIV replication and responsiveness to therapy)
RN   16561-29-8  CAPLUS
CN   Tetradecanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-9a-(acetyloxy)-
     1a,1b,4,4a,5,7a,7b,8,9,9a-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-
```

1,1,6,8-tetramethyl-5-oxo-1H-cyclopropa[3,4]benz[1,2-e]azulen-9-yl ester
(CA INDEX NAME)

Absolute stereochemistry.



=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	55.94	375.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.74	-5.74

FILE 'REGISTRY' ENTERED AT 15:01:45 ON 08 JUL 2009

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 7 JUL 2009 HIGHEST RN 1161069-81-3
DICTIONARY FILE UPDATES: 7 JUL 2009 HIGHEST RN 1161069-81-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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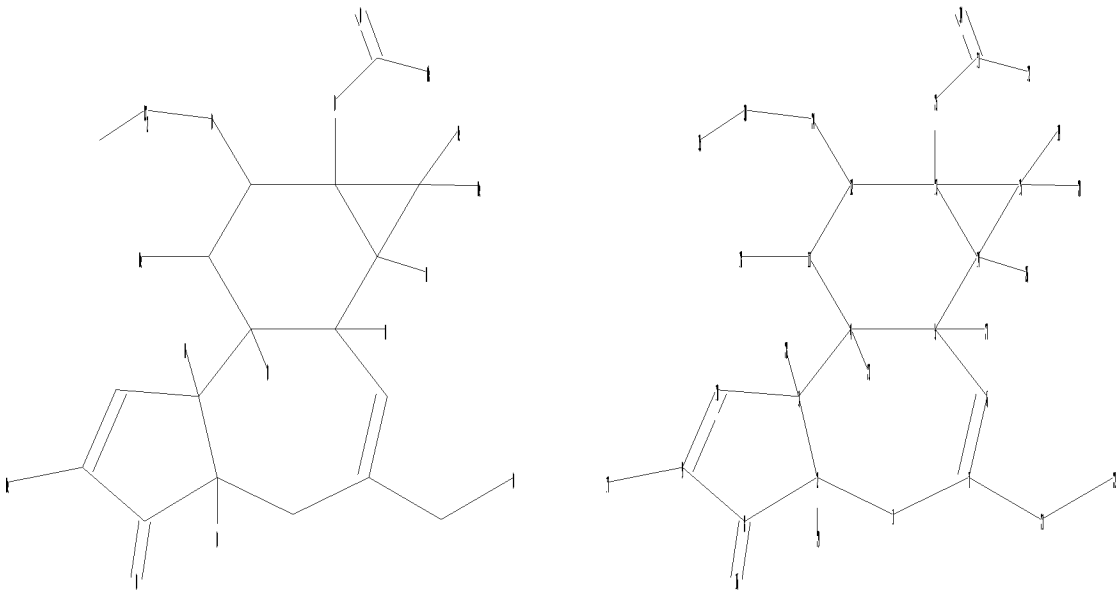

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ring nodes :
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chain bonds :
2-29 3-28 4-23 5-27 7-21 8-16 9-17 11-18 12-24 13-25 14-26 15-19 15-20
21-22 24-30 25-31 30-35 31-32 31-34
ring bonds :
1-2 1-7 2-3 2-8 3-4 3-10 4-5 4-11 5-6 5-14 6-7 8-9 9-10 11-12 12-13
13-14 13-15 14-15
exact/norm bonds :
1-2 1-7 2-3 2-8 2-29 3-4 3-10 4-5 4-11 4-23 5-6 5-14 6-7 8-9 8-16
9-10 11-12 12-13 12-24 13-14 13-15 13-25 14-15 21-22 25-31 31-32 31-34
exact bonds :
3-28 5-27 7-21 9-17 11-18 14-26 15-19 15-20 24-30 30-35

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 34:CLASS 35:CLASS

L14 STRUCTURE UPLOADED

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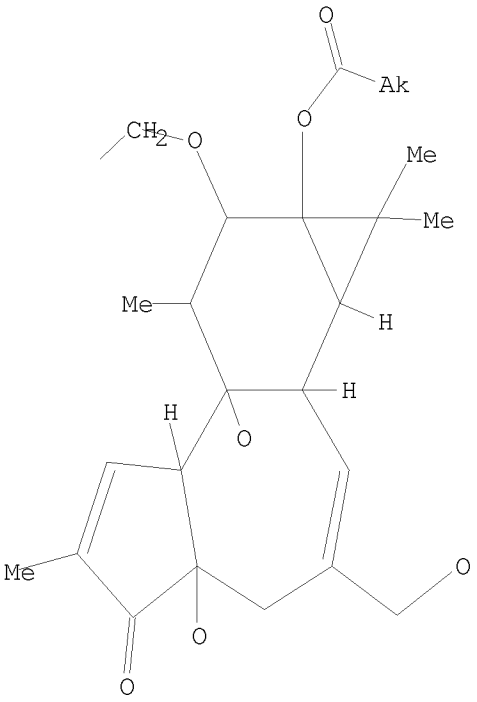
L14 HAS NO ANSWERS
L14 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l14 sub=l5 sss ful
FULL SUBSET SEARCH INITIATED 15:02:28 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 687 TO ITERATE

100.0% PROCESSED 687 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

L15 4 SEA SUB=L5 SSS FUL L14

=> fil cap

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	44.48	420.44

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.74

FILE 'CAPLUS' ENTERED AT 15:02:32 ON 08 JUL 2009

FILE COVERS 1907 - 8 Jul 2009 VOL 151 ISS 2
FILE LAST UPDATED: 7 Jul 2009 (20090707/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

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YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

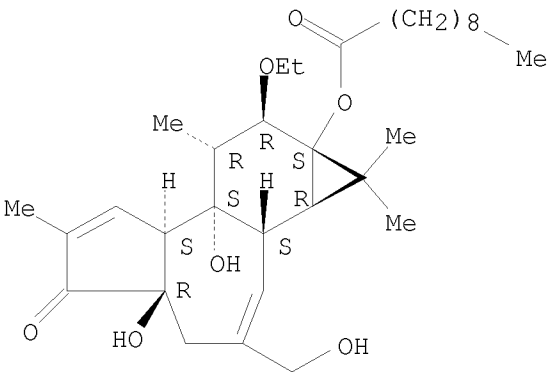
=> s l15
L16 5 L15

=> d l16 1-5 ibib abs hitstr

L16 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:520769 CAPLUS
DOCUMENT NUMBER: 143:145807
TITLE: Synthesis of new phorbol derivatives having ethereal side chain and evaluation of their anti-HIV activity
AUTHOR(S): Matsuya, Yuji; Yu, Zhong; Yamamoto, Naoki; Mori, Masao; Saito, Haruo; Takeuchi, Makoto; Ito, Mamiko; Nemoto, Hideo
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Toyama Medical and Pharmaceutical University, Toyama, 930-0914, Japan
SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(14), 4383-4388
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:145807
AB Several new phorbol derivs. having ethereal substituents at the 12-position were synthesized and subjected to biol. evaluation to find new candidates of an anti-HIV agent. Among them, 12-O-(methoxymethyl)phorbol 13-decanoate showed potent inhibitory activity against infection of HIV-1 in MT-4 cells (EC50: 1.3 ng/mL) and relatively low cytotoxicity (CC50: 8.3 μg/mL). This compound was also found to have sufficient stability in mouse plasma compared with the corresponding 12-acetate derivative, which was an equipotent HIV-1 inhibitor, but with an activity that decreased considerably after plasma treatment.
IT 800385-94-8P
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of new phorbol derivs. having ethereal side chain and evaluation of their anti-HIV activity)
RN 800385-94-8 CAPLUS

CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-9-ethoxy-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (CA INDEX NAME)

Absolute stereochemistry.

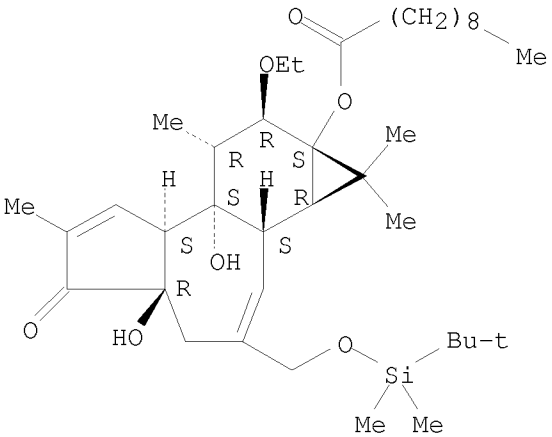


IT 800385-90-4P, 12-O-Ethyl-20-O-(tert-butyldimethylsilyl)phorbol 13-decanoate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of new phorbol derivs. having ethereal side chain and evaluation of their anti-HIV activity)

RN 800385-90-4 CAPLUS

CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-9-ethoxy-1,1a,1b,4,4a,5,7a,7b,9,9-decahydro-4a,7b-dihydroxy-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:1036894 CAPLUS
DOCUMENT NUMBER: 142:16778
TITLE: Compounds and preparations having antiviral effect
INVENTOR(S): Mori, Masao; Saito, Haruo; Nemoto, Hideo; Yamamoto, Naoki; Hattori, Masao

PATENT ASSIGNEE(S): Lead Chemical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004103360	A1	20041202	WO 2003-JP6422	20030522
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003242405	A1	20041213	AU 2003-242405	20030522
US 20070066684	A1	20070322	US 2005-557922	20051222

PRIORITY APPLN. INFO.: WO 2003-JP6422 A 20030522
OTHER SOURCE(S): MARPAT 142:16778
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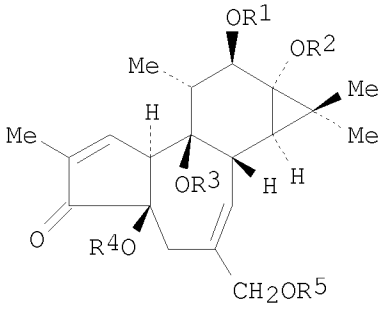


I

AB Antiviral prepns. containing, as the active ingredient, phorbol derivs. which are represented by the following general formula I: wherein R1 represents -CH2aX(CH2)bCH3, -CH2cX(CH2)dYCH3, -CO(CH2)eCH3or -(CH2)fCH3; R2 represents -CO(CH2)nCH3; and R3, R4 and R5 represent each hydrogen or aliphatic or aromatic carboxylate (wherein X and Y are each O or S; and a to f and n stand for each a numerical value); and show a specific safety index S.I. = EC50/EC50 (i.e., a ratio of the concentration at which HIV-1-induced cytopathogenic effect (CPE) in MT-4 cells is inhibited by 50% to the concentration at which the survival of MT-4 cells is lowered by 50% in a cell proliferation test) of 10 or more. These prepns. are efficacious particularly against human immunodeficiency virus (HIV).

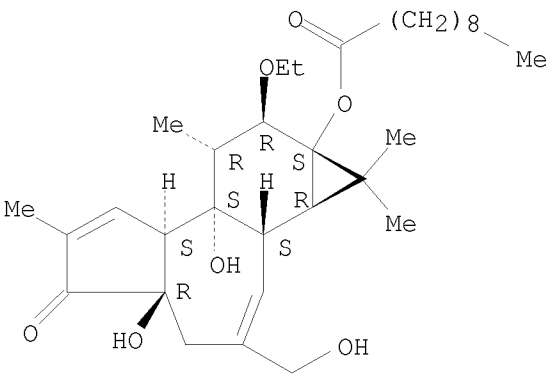
IT 800385-94-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(phorbol compds. and prepns. having antiviral effect against HIV)

RN 800385-94-8 CAPLUS

CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-9-ethoxy-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester

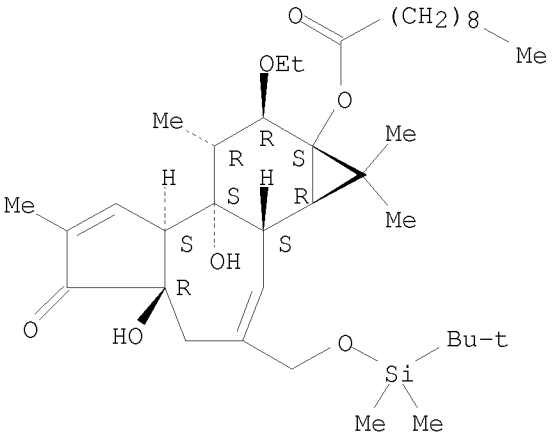
(CA INDEX NAME)

Absolute stereochemistry.



IT 800385-90-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(phorbol compds. and prepns. having antiviral effect against HIV)
RN 800385-90-4 CAPLUS
CN Decanoic acid, (1aR,1bS,4aR,7aS,7bS,8R,9R,9aS)-3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-9-ethoxy-1,1a,1b,4,4a,5,7a,7b,9,9-decahydro-4a,7b-dihydroxy-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester (9CI) (CA INDEX NAME)

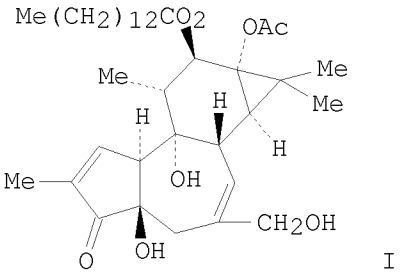
Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1979:518341 CAPLUS
DOCUMENT NUMBER: 91:118341
ORIGINAL REFERENCE NO.: 91:19036h,19037a
TITLE: Stimulation of choline incorporation in cell cultures by phorbol derivatives and its correlation with their irritant and tumor-promoting activity
AUTHOR(S): Kinzel, Volker; Kreibich, Gert; Hecker, Erich; Suess, Rudolf
CORPORATE SOURCE: Inst. Exp. Pathol., Dtsch. Krebsforschungszent., Heidelberg, D-6900, Fed. Rep. Ger.

SOURCE: Cancer Research (1979), 39(7, Pt. 1), 2743-50
CODEN: CNREA8; ISSN: 0008-5472
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

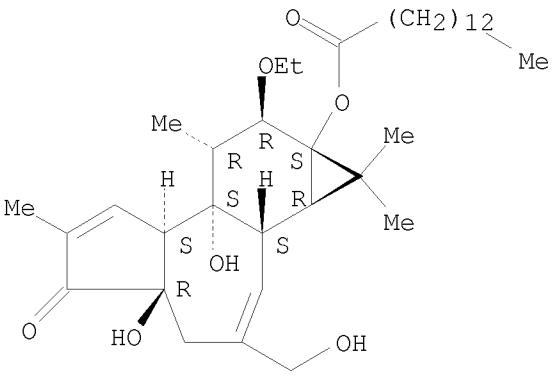
AB An increasing choline [62-49-7] incorporation into phosphatidylcholine was observed when HeLa and other lines of cells (as monolayers or suspension) were treated with low concns. (10-9-10-8 M) of 12-O-tetradecanoylphorbol 13-acetate (I) [16561-29-8]. Increasing concns. of I applied to cells produced rapid maximal incorporation rates. This effect of I was also observed when cells were preincubated with radioactive choline, thereby excluding the possibility that I changed only the permeability for the radioactive precursor. Metabolic inhibitors of RNA and protein synthesis have little effect on choline incorporation, suggesting a direct activation of the phospholipid metabolism by I. Tosylphenylalaninechloromethyl ketone [402-71-1], which was shown to inhibit the inflammatory and tumor-promoting effect of I on the mouse ear, did not influence the choline response to I in HeLa cells. Colchicine [64-86-8] sensitized HeLa cells to the effect of I, leading to a further increase in the choline incorporation rate. Cultivation of HeLa cells in the prolonged presence of I did not change their response to the phorbol ester. Using choline incorporation in HeLa cells as a standard assay, a large number of phorbol derivs. were tested in concentration series covering several orders of magnitude. The lowest concentration of a particular phorbol ester required to elicit after 5 h a 2-fold increased in the choline incorporation correlated well with the irritant activity of these compds. on mouse ear. Structurally different tumor promoters (such as mezerein [34807-41-5], cantharidin [56-25-7], and anthralin [480-22-8] did not elicit a significant response in the standard assay using HeLa cells.

IT 37558-20-6
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (carcinogenicity of, choline incorporation in HeLa cells in relation to)

RN 37558-20-6 CAPLUS

CN Tetradecanoic acid, 9-ethoxy-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester, [1aR-(1aα,1bβ,4aβ,7aα,7bα,8α,9β,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

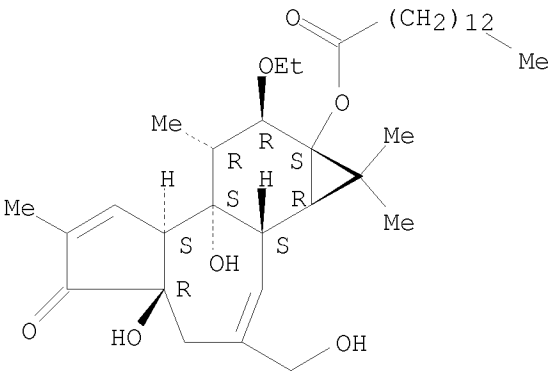


L16 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1972:484233 CAPLUS
DOCUMENT NUMBER: 77:84233
ORIGINAL REFERENCE NO.: 77:13869a,13872a
TITLE: Effect of the biologically active phorbol ester on HeLa cells
AUTHOR(S): Suess, R.; Kinzel, V.; Kreibich, G.
CORPORATE SOURCE: Inst. Exp. Pathol., Dtsch. Krebsforschungszent., Heidelberg, Fed. Rep. Ger.
SOURCE: Aktuel. Probl. Geb. Cancerol., Heidelberg. Symp., 3rd (1971), Meeting Date 1970, 109-14. Editor(s): Lettre, H. Springer: Berlin, Ger.
CODEN: 25DMAG
DOCUMENT TYPE: Conference
LANGUAGE: German

AB The cocarcinogens 12-O-tetradecanoylphorbol 13-acetate (I) [16561-29-8] and phorbol 12,13-didecanoate (II) [24928-17-4] inhibited incorporation of labeled thymidine into DNA of HeLa cells in a concentration-dependent manner, but with a plateau over the range 10-8-10-6 M within which incorporation was independent of phorbol ester concentration The noncocarcinogenic isomer 4α-phorbol 12,13-didecanoate (III) [27536-56-7] inhibited thymidine incorporation without a plateau. I and II stimulated incorporation of choline into membrane lipids of HeLa cells, whereas III did not. Other phorbol derivs. as well were either active in all test systems (cocarcinogenesis, inflammation, thymidine and choline incorporation) or inactive in all. Active compounds may block cells from entering the S phase of the cell cycle.

IT 37558-20-6
RL: BIOL (Biological study)
(DNA and lipid formation by HeLa cells in response to, carcinogenicity in relation to)
RN 37558-20-6 CAPLUS
CN Tetradecanoic acid, 9-ethoxy-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-4a,7b-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-9aH-cyclopropa[3,4]benz[1,2-e]azulen-9a-yl ester, [1aR-(1aα,1bβ,4aβ,7aα,7bα,8α,9β,9a.alpha.)]- (9CI) (CA INDEX NAME)

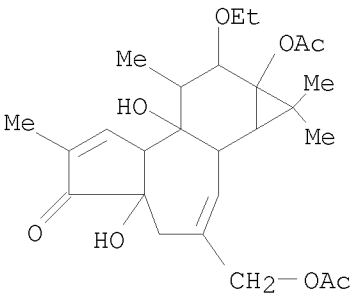
Absolute stereochemistry.



L16 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:47626 CAPLUS
DOCUMENT NUMBER: 70:47626
ORIGINAL REFERENCE NO.: 70:8958h,8959a
TITLE: Chemistry of phorbol. V. Phorbol ethers
AUTHOR(S): Kreibich, Gert; Hecker, Erich
CORPORATE SOURCE: Biochem. Inst., Deut. Krebsforschungszentrums, Heidelberg, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie, Biochemie, Biophysik, Biologie (1968), 23(11), 1444-52
CODEN: ZENBAX; ISSN: 0044-3174
DOCUMENT TYPE: Journal
LANGUAGE: German

AB Phorbol 12,13-diacetate was treated with CH2N2 and (iso-PrO)3Al to give 70% 12,13-di-O-acetylphorbol 20-Me ether (I), m. 196-8°. Similarly prepared were 9,12,13-tri-O-acetylphorbol 20-Me ether (which was peracetylated to 74% phorbol pentaacetate), phorbol 13,20-di-Me ether, [α]25578 80° (1%, dioxane), yield 42%; 13-O-methylphorbol 20-trityl ether; and 4,20-di-O-methylphorbol 12,13-diacetate. I was also obtained in 50% yield by treating phorbol 12,13-diacetate with MeI-Ag2O in AcOEt. Similarly prepared were didehydrophorbol 12,20-diacetate, m. 186-9°, 4-O-methylphorbol 13,20-diacetate, yield 45%; and 4-O-methylphorbol 12,13,20-triacetate (II), [α]25578 73° (1%, dioxane). Phorbol 20-trityl ether reacted with MeCHN2 and (iso-PrO)3Al to give 19% 12-O-ethylphorbol 20-trityl ether and 52% 13-O-ethylphorbol 20-trityl ether, m. 128-30°. Oxidation of phorbol 12,20-diacetate with PbO2 gave 30% didehydrophorbol 12,20-diacetate and a resinous by-product. 12-O-Ethylphorbol 20-trityl ether was hydrolyzed with HOAc to give 70% phorbol 12-Et ether, which was acetylated to 76% 12-O-ethylphorbol 13,20-diacetate, m. 189-91°. II was similarly prepared in 92% yield. II was treated with 60% HClO4 to give 4-O-methylphorbol 12,13-diacetate. 4,13-Di-O-methylphorbol 12,20-diacetate was similarly prepared in 28% yield. N.M.R., uv, and ir spectral data are reported.

IT 22376-28-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 22376-28-9 CAPLUS
CN 5H-Cyclopropa[3,4]benz[1,2-e]azulen-5-one, 9β-ethoxy-1,1aα,1bβ,4,4a,7aα,7b,8,9,9a-decahydro-4aβ,7bα,9aα-trihydroxy-3-(hydroxymethyl)-1,1,6,8α-tetramethyl-, 3,9a-diacetate, (+)- (8CI) (CA INDEX NAME)

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